Numerical Acceleration of Three-Dimensional Quantum Transport Method Using a Seven-Diagonal Preconditioner

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The exactly solvable, real-space, open-boundary planar supercell stack method (OPSSM) has been applied to a variety of topics involving 3D quantum transport in mesoscopic devices [1]. OPSSM formulates quantum mechanical scattering problems for supercell geometries as sparse non-Hermitian linear systems, and solve them iteratively by the Quasi-Minimal Residual (QMR) method [2]. Recently we demonstrated that the convergence rate of our method could be greatly accelerated using a seven-diagonal pre-conditioner. Table 1 illustrates performance gains achieved in typical applications involving MOS tunnel structures and GaAs/AlAs double barrier heterostructures (DBHs). With over two orders of magnitude of numerical acceleration, we are now able to obtain more accurate results by using larger supercells. In particular, supercell periodic boundary condition induced artifacts in the transmission coefficient spectrum of a double barrier structure with interface roughness [3] are reduced significantly. We will also discuss results on studies of interface roughness effects and dielectric breakdown in n^+ poly-Si/SiO_2/p-Si tunnel structures containing ultra-thin oxide layers [4, 5].

Table 1. Speed-up obtained in typical 3D scattering calculations with a 7-diagonal pre-conditioner.

	No Pre-conditioner	7-Diagonal Preconditioner	Speed-Up
DBH 16x16x26	8.92 h	1.66 h	5.4
DBH 32x32x26	208.7 h	17.6 h	12
DBH 64x64x26	1511 h (Poor Convergence)	283.2 h (Good Convergence)	>> 5
MOS 64x64x37 (Tol=1E-10)	1618.5 h	23.2 h	70
MOS 64x64x37	1618.5 h (Tol=1E-10)	5.7 h (Tol=1E-7)	284

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